



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:08 AM UTC

PDB ID : 1YTO / pdb_00001yto
Title : Crystal Structure of Gly19 deletion Mutant of Human Acidic Fibroblast Growth Factor
Authors : Lee, J.; Blaber, M.
Deposited on : 2005-02-10
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

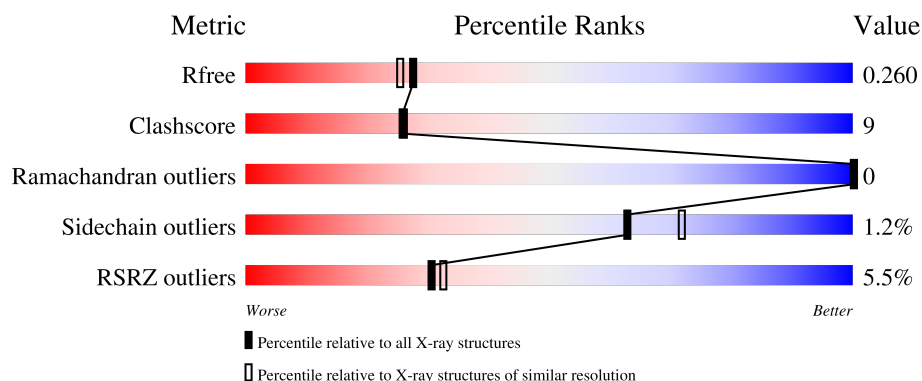
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	145	8% 75% 20% • •
1	B	145	8% 82% 14% • •
1	C	145	9% 79% 19% •
1	D	145	3% 76% 17% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMT	A	1160	-	X	-	-
3	FMT	C	1161	-	X	-	-
3	FMT	D	1162	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4777 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Heparin-binding growth factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1122	712	199	207	4			
1	B	141	Total	C	N	O	S	0	0	0
			1142	724	205	209	4			
1	C	141	Total	C	N	O	S	0	0	0
			1142	724	205	209	4			
1	D	138	Total	C	N	O	S	0	0	0
			1112	706	196	206	4			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1D	HIS	-	expression tag	UNP P05230
A	1D	HIS	-	expression tag	UNP P05230
A	1D	HIS	-	expression tag	UNP P05230
A	1D	HIS	-	expression tag	UNP P05230
A	1E	HIS	-	expression tag	UNP P05230
A	1F	HIS	-	expression tag	UNP P05230
A	?	-	GLY	deletion	UNP P05230
B	1B	HIS	-	expression tag	UNP P05230
B	1B	HIS	-	expression tag	UNP P05230
B	1C	HIS	-	expression tag	UNP P05230
B	1D	HIS	-	expression tag	UNP P05230
B	1E	HIS	-	expression tag	UNP P05230
B	1F	HIS	-	expression tag	UNP P05230
B	?	-	GLY	deletion	UNP P05230
C	1B	HIS	-	expression tag	UNP P05230
C	1B	HIS	-	expression tag	UNP P05230
C	1C	HIS	-	expression tag	UNP P05230
C	1D	HIS	-	expression tag	UNP P05230
C	1E	HIS	-	expression tag	UNP P05230
C	1F	HIS	-	expression tag	UNP P05230
C	?	-	GLY	deletion	UNP P05230

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1E	HIS	-	expression tag	UNP P05230
D	1E	HIS	-	expression tag	UNP P05230
D	1E	HIS	-	expression tag	UNP P05230
D	1E	HIS	-	expression tag	UNP P05230
D	1E	HIS	-	expression tag	UNP P05230
D	1F	HIS	-	expression tag	UNP P05230
D	?	-	GLY	deletion	UNP P05230

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	51	Total	O	0	0
			51	51		
4	C	53	Total	O	0	0
			53	53		
4	D	54	Total	O	0	0
			54	54		

- Molecule 1: Heparin-binding growth factor 1



-

-
- SER
 ASP
 ASP
 SER
 HIS
- G6 N7 Y8 K9 K10 P11 K12 L13 N18 F22 L26 F27 T30 R35 D36 R37 A66 M67 D68 L72 L73 Q77 N95 E104 V109 G110 L111 K112 K113 N114 R119 R122 T123 H124 Q127 A128 A129 L133 V137

-
- ASP
- SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.39Å 109.17Å 68.98Å 90.00° 107.19° 90.00°	Depositor
Resolution (Å)	49.10 – 2.10 49.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.10-2.10) 95.3 (49.10-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.32 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.250 0.206 , 0.260	Depositor DCC
R_{free} test set	2083 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4777	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/1152	0.94	3/1557 (0.2%)
1	B	0.49	0/1174	0.91	3/1587 (0.2%)
1	C	0.47	0/1174	0.86	2/1587 (0.1%)
1	D	0.49	0/1141	0.88	3/1542 (0.2%)
All	All	0.49	0/4641	0.90	11/6273 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	VAL	N-CA-C	-7.89	98.48	108.89
1	C	109	VAL	N-CA-C	-7.60	98.85	108.89
1	A	55	TYR	N-CA-C	-7.57	97.92	109.95
1	A	109	VAL	N-CA-C	-7.31	99.24	108.89
1	D	109	VAL	N-CA-C	-6.91	99.76	108.89
1	A	49	GLU	N-CA-C	-6.07	97.87	110.80
1	C	13	LEU	N-CA-C	-5.80	100.73	109.95
1	B	55	TYR	N-CA-C	-5.65	100.50	109.59
1	D	55	TYR	N-CA-C	-5.36	100.67	109.40
1	D	49	GLU	N-CA-C	-5.24	106.03	112.90
1	B	49	GLU	N-CA-C	-5.05	100.05	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1122	0	1099	34	0
1	B	1142	0	1113	14	0
1	C	1142	0	1113	18	0
1	D	1112	0	1092	21	1
2	A	10	0	0	0	0
2	D	10	0	0	0	0
3	A	3	0	2	0	0
3	C	3	0	2	0	0
3	D	3	0	2	0	0
4	A	72	0	0	7	0
4	B	51	0	0	2	0
4	C	53	0	0	3	1
4	D	54	0	0	1	0
All	All	4777	0	4423	85	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:PRO:HB2	1:D:7:ASN:HD21	1.31	0.94
1:B:117:CYS:HB2	4:B:708:HOH:O	1.70	0.89
1:A:12:LYS:NZ	1:A:46:LEU:HD13	1.95	0.80
1:A:12:LYS:H	1:A:12:LYS:HE2	1.52	0.75
1:A:81:GLU:HG3	1:A:101:LYS:HD2	1.71	0.73
1:A:12:LYS:HE2	1:A:12:LYS:N	2.06	0.70
1:C:9:LYS:HD2	1:C:9:LYS:H	1.57	0.69
1:A:1(F):HIS:CD2	1:A:2:ASN:HD22	2.15	0.65
1:A:1(D):HIS:HA	4:A:731:HOH:O	1.99	0.61
1:D:5:PRO:HB2	1:D:7:ASN:ND2	2.12	0.60
1:A:137:VAL:HG22	4:A:645:HOH:O	2.01	0.58
1:A:12:LYS:CE	1:A:46:LEU:HD13	2.34	0.58
1:D:9:LYS:HD2	1:D:10:LYS:HG3	1.86	0.57
1:D:16:CYS:HB2	1:D:132:PHE:CE2	2.40	0.57
1:D:12:LYS:HG3	4:D:641:HOH:O	2.04	0.57
1:A:1(F):HIS:CD2	1:A:2:ASN:H	2.23	0.56
1:C:119:ARG:HB2	1:C:122:ARG:HG2	1.88	0.56
1:A:12:LYS:HB2	1:A:135:LEU:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:GLU:H	1:C:104:GLU:CD	2.15	0.55
1:B:104:GLU:H	1:B:104:GLU:CD	2.15	0.55
1:A:12:LYS:HZ2	1:A:46:LEU:HD13	1.70	0.54
1:A:1(D):HIS:N	4:A:731:HOH:O	2.39	0.54
1:C:6:GLY:C	1:C:9:LYS:HZ2	2.16	0.54
1:A:81:GLU:HB3	4:A:711:HOH:O	2.08	0.53
1:A:57:LYS:HE2	1:A:64:TYR:CZ	2.44	0.53
1:A:1(F):HIS:HD2	1:A:2:ASN:H	1.55	0.53
1:A:1(E):HIS:HE1	1:A:103:ALA:O	1.92	0.53
1:B:29:GLY:HA3	4:B:606:HOH:O	2.07	0.53
1:D:10:LYS:HB2	1:D:10:LYS:NZ	2.26	0.51
1:B:133:LEU:O	1:B:135:LEU:HD22	2.11	0.50
1:A:1(D):HIS:CA	4:A:731:HOH:O	2.58	0.50
1:A:12:LYS:HE2	1:A:12:LYS:CA	2.41	0.50
1:A:58:SER:OG	4:A:624:HOH:O	2.20	0.49
1:B:8:TYR:CE2	1:B:48:ALA:HB2	2.47	0.49
1:B:72:LEU:HD22	1:D:122:ARG:CZ	2.43	0.49
1:C:66:ALA:O	1:C:73:LEU:HA	2.13	0.49
1:C:10:LYS:HB3	1:C:11:PRO:HD2	1.96	0.48
1:C:9:LYS:HB2	4:C:677:HOH:O	2.14	0.48
1:C:137:VAL:HG22	4:C:693:HOH:O	2.14	0.48
1:A:12:LYS:NZ	1:A:46:LEU:CD1	2.72	0.47
1:C:124:HIS:CE1	1:C:127:GLN:HE21	2.32	0.47
1:B:112:LYS:HD3	1:B:116:SER:OG	2.15	0.46
1:D:31:VAL:HG12	1:D:117:CYS:SG	2.56	0.46
1:D:118:LYS:HE3	1:D:122:ARG:O	2.16	0.46
1:D:40:GLN:O	1:D:40:GLN:HG2	2.16	0.45
1:C:22:PHE:CE2	1:C:37:ARG:HG2	2.51	0.45
1:C:124:HIS:CE1	1:C:127:GLN:NE2	2.85	0.45
1:C:68:ASP:HB2	4:C:549:HOH:O	2.17	0.45
1:B:123:THR:HA	1:B:127:GLN:OE1	2.17	0.44
1:C:18:ASN:ND2	1:C:111:LEU:O	2.50	0.44
1:B:124:HIS:HD2	1:B:125:TYR:O	2.01	0.44
1:D:87:GLU:HG3	1:D:97:TYR:CE1	2.52	0.44
1:A:1(F):HIS:HD2	1:A:2:ASN:HD22	1.63	0.43
1:D:81:GLU:HG3	1:D:101:LYS:HD2	2.00	0.43
1:D:104:GLU:H	1:D:104:GLU:CD	2.25	0.43
1:C:7:ASN:HD21	1:C:95:ASN:HD21	1.66	0.43
1:C:9:LYS:H	1:C:9:LYS:CD	2.27	0.43
1:A:68:ASP:HB2	4:A:604:HOH:O	2.18	0.43
1:D:118:LYS:HE2	1:D:127:GLN:NE2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LEU:HA	1:D:55:TYR:O	2.19	0.43
1:D:122:ARG:HA	1:D:122:ARG:HD3	1.86	0.43
1:D:49:GLU:OE1	1:D:55:TYR:HE2	2.02	0.42
1:B:8:TYR:HB3	1:B:46:LEU:O	2.19	0.42
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.93	0.42
1:C:18:ASN:ND2	1:C:129:ALA:HA	2.34	0.42
1:A:12:LYS:HZ1	1:A:46:LEU:CD1	2.32	0.42
1:B:102:HIS:HA	1:B:104:GLU:OE2	2.20	0.42
1:A:104:GLU:CD	1:A:104:GLU:H	2.28	0.42
1:D:66:ALA:O	1:D:73:LEU:HA	2.19	0.42
1:A:63:GLN:HG2	1:A:77:GLN:OE1	2.20	0.42
1:A:133:LEU:HD12	1:A:133:LEU:HA	1.90	0.41
1:B:15:TYR:HB3	1:B:135:LEU:HD21	2.01	0.41
1:D:10:LYS:HB2	1:D:10:LYS:HZ2	1.84	0.41
1:A:39:ASP:O	1:A:42:ILE:HG12	2.20	0.41
1:B:118:LYS:HE3	1:B:122:ARG:O	2.21	0.41
1:A:12:LYS:HA	1:A:137:VAL:HG13	2.01	0.41
1:A:68:ASP:OD1	1:A:68:ASP:C	2.64	0.41
1:A:122:ARG:HD2	1:C:72:LEU:HD12	2.02	0.41
1:A:66:ALA:O	1:A:73:LEU:HA	2.20	0.41
1:D:102:HIS:HB3	1:D:105:LYS:HE2	2.02	0.40
1:A:12:LYS:NZ	1:A:44:LEU:O	2.54	0.40
1:C:112:LYS:HE3	1:C:114:ASN:HD21	1.85	0.40
1:D:1(E):HIS:HE1	1:D:106:ASN:OD1	2.04	0.40
1:A:8:TYR:HB3	1:A:46:LEU:O	2.21	0.40
1:A:64:TYR:CE1	1:A:79:PRO:HD3	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1(E):HIS:N	4:C:707:HOH:O[2_746]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	137/145 (94%)	131 (96%)	6 (4%)	0	100	100
1	B	139/145 (96%)	131 (94%)	8 (6%)	0	100	100
1	C	139/145 (96%)	131 (94%)	8 (6%)	0	100	100
1	D	136/145 (94%)	129 (95%)	7 (5%)	0	100	100
All	All	551/580 (95%)	522 (95%)	29 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	123/129 (95%)	122 (99%)	1 (1%)	73	81
1	B	125/129 (97%)	124 (99%)	1 (1%)	73	81
1	C	125/129 (97%)	123 (98%)	2 (2%)	55	64
1	D	122/129 (95%)	120 (98%)	2 (2%)	55	64
All	All	495/516 (96%)	489 (99%)	6 (1%)	63	72

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	B	133	LEU
1	C	77	GLN
1	C	133	LEU
1	D	9	LYS
1	D	10	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1(F)	HIS
1	A	2	ASN
1	A	41	HIS
1	A	45	GLN
1	A	92	ASN
1	B	2	ASN
1	B	21	HIS
1	B	43	GLN
1	B	45	GLN
1	B	92	ASN
1	B	124	HIS
1	C	1(B)	HIS
1	C	7	ASN
1	C	18	ASN
1	C	21	HIS
1	C	92	ASN
1	C	127	GLN
1	D	2	ASN
1	D	7	ASN
1	D	77	GLN
1	D	93	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FMT	A	1160	-	2,2,2	5.35	2 (100%)	1,1,1	1.36	0
2	SO4	D	202	-	4,4,4	0.37	0	6,6,6	0.15	0
2	SO4	A	200	-	4,4,4	0.39	0	6,6,6	0.11	0
2	SO4	A	201	-	4,4,4	0.37	0	6,6,6	0.15	0
2	SO4	D	203	-	4,4,4	0.40	0	6,6,6	0.12	0
3	FMT	C	1161	-	2,2,2	5.46	2 (100%)	1,1,1	1.28	0
3	FMT	D	1162	-	2,2,2	5.46	2 (100%)	1,1,1	1.28	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1162	FMT	O1-C	5.58	1.53	1.22
3	C	1161	FMT	O1-C	5.56	1.52	1.22
3	A	1160	FMT	O1-C	5.48	1.52	1.22
3	C	1161	FMT	O2-C	5.36	1.56	1.28
3	D	1162	FMT	O2-C	5.34	1.55	1.28
3	A	1160	FMT	O2-C	5.22	1.55	1.28

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	139/145 (95%)	-0.03	2 (1%) 73 75	20, 31, 51, 65	0
1	B	141/145 (97%)	0.32	11 (7%) 19 20	20, 33, 62, 75	0
1	C	141/145 (97%)	0.40	13 (9%) 14 15	20, 37, 64, 74	0
1	D	138/145 (95%)	0.26	5 (3%) 46 48	22, 34, 59, 71	0
All	All	559/580 (96%)	0.24	31 (5%) 30 32	20, 33, 61, 75	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	VAL	7.8
1	A	1(D)	HIS	3.5
1	C	6	GLY	3.4
1	B	1(D)	HIS	3.4
1	B	6	GLY	3.3
1	C	30	THR	3.3
1	B	1(C)	HIS	3.3
1	C	37	ARG	3.3
1	C	122	ARG	3.3
1	D	137	VAL	3.1
1	D	9	LYS	3.0
1	C	7	ASN	2.6
1	B	30	THR	2.5
1	B	1(B)	HIS	2.5
1	B	37	ARG	2.4
1	B	122	ARG	2.3
1	C	27	PRO	2.3
1	C	77	GLN	2.3
1	C	1(D)	HIS	2.3
1	A	137	VAL	2.2
1	C	35	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	7	ASN	2.2
1	C	1(C)	HIS	2.2
1	B	13	LEU	2.2
1	B	124	HIS	2.1
1	C	113	LYS	2.1
1	D	10	LYS	2.1
1	C	26	LEU	2.0
1	D	124	HIS	2.0
1	C	9	LYS	2.0
1	B	113	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	200	5/5	0.79	0.18	78,82,87,89	0
2	SO4	D	203	5/5	0.81	0.18	73,80,88,91	0
3	FMT	A	1160	3/3	0.84	0.13	42,42,49,51	0
2	SO4	A	201	5/5	0.90	0.15	81,82,85,91	0
3	FMT	C	1161	3/3	0.92	0.11	38,38,47,50	0
2	SO4	D	202	5/5	0.93	0.17	48,51,63,69	0
3	FMT	D	1162	3/3	0.94	0.10	33,33,45,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.